



| The European Synchrotron

FACING THE CHALLENGES OF EXPERIMENT CONTROL AND DATA MANAGEMENT AT ESRF-EBS



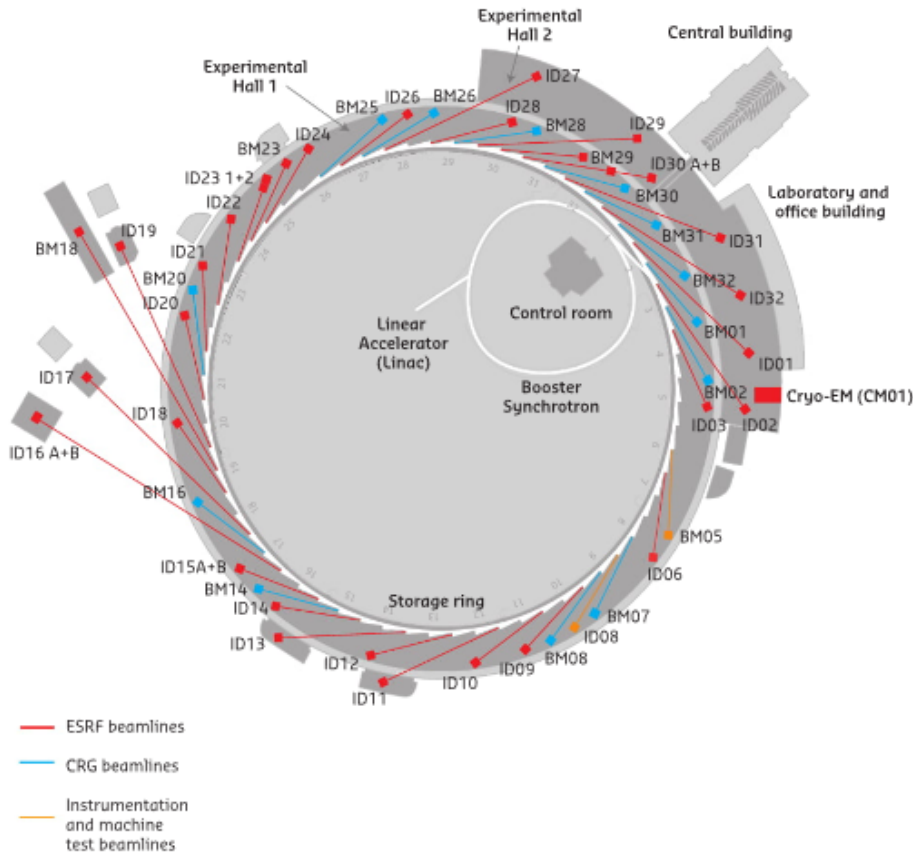
Outline

- **The Challenges**
- **Data Acquisition**
- **Online Data Analysis**
- **Conclusion**

Jens Meyer on behalf of the ESRF Software Group

ESRF BEAMLINES AND EXPERIMENT TYPES

33 ESRF beamlines and 13 CRG beamlines



SOURCE POSITION	INDEPENDENT END-STATIONS	FIELD OF RESEARCH	STATUS	DATE
ID01	1	Microdiffraction imaging	Operational	Since 12/14
ID02	1	Time-resolved ultrasmall-angle X-ray scattering	Operational	Since 07/14
ID03	1	Hard X-ray diffraction microscopy	Construction	
ID06	1	Large volume press /Hard X-ray diffraction microscopy	Operational	Since 10/13
ID09	1	Time-resolved structural dynamics	Operational	Since 09/94
ID10	1	Soft interfaces and coherent scattering	Operational	Since 06/12
ID11	1	Materials science	Operational	Since 09/94
ID12	1	Polarisation-dependent X-ray spectroscopy	Operational	Since 01/95
ID13	1	Microfocus	Operational	Since 09/94
ID14	1	Nuclear scattering	Construction	
ID15A	0.85	Materials chemistry and engineering	Operational	Since 11/16
ID15B	0.5	High-pressure diffraction	Operational	Since 11/16
ID16A	1	Nano-imaging	Operational	Since 05/14
ID16B	1	Nano-analysis	Operational	Since 04/14
ID17	1	Medical	Operational	Since 05/97
ID18	1	Nuclear scattering	Operational	Since 01/96
ID19	1	Microtomography	Operational	Since 06/96
ID20	1	Inelastic X-ray scattering	Operational	Since 06/13
ID21	1	X-ray microscopy / IR spectroscopy	Operational	Since 12/97
ID22	1	High resolution powder diffraction	Operational	Since 05/14
ID23	2	Macromolecular crystallography MAD	Operational	Since 06/04
		Macromolecular crystallography microfocus	Operational	Since 09/05
ID24	0.5	Dispersive EXAFS	Operational	Since 12/21
ID26	1	X-ray absorption and emission	Operational	Since 11/97
ID27	1	High pressure	Operational	Since 11/21
ID28	1	X-ray scattering II	Operational	Since 12/98
ID29	1	Multiwavelength anomalous diffraction	Closed	Since 08/20
ID30A	2	Macromolecular crystallography	Operational	Since 07/14
ID30B	1	Macromolecular crystallography	Operational	Since 04/15
ID31	1	Interfaces and materials processing	Operational	Since 11/15
ID32	1	Soft X-ray spectroscopy	Operational	Since 11/14
BM18	1	Hierarchical tomography	Construction	Since 12/14
BM23	1	X-ray absorption spectroscopy	Operational	Since 01/21
BM29	1	Bio SAXS	Operational	Since 06/12
CM01	1	Cryo-EM	Operational	Since 11/17

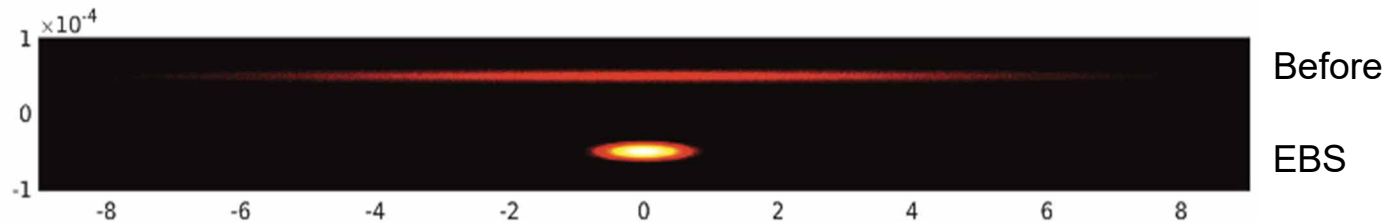
46 Beamlines
More than 100 scientific techniques

ESRF-EBS

The **first fourth generation high-energy synchrotron** (Hybrid Multi-Bend Achromat)

Shutdown December 2018 and back to user operation September 2020

X-ray beam is **100 times more brilliant and coherent** than before



Much higher photon flux on the sample, to do experiments

- 10 to 100 times faster data acquisition
- Much higher data rates

The Software Requirements for ESRF-EBS

Data acquisition in the kHz and up to the MHz range

Data reduction as early as possible to reduce the amount of raw data to store

Automated online data analysis

Online data visualization for data validation

Management of experiments raw data, meta data and processed data



WE3BCO07 Extending the ICAT metadata catalogue to new scientific use cases

Command line driven sequencer written in Python

Main concepts:

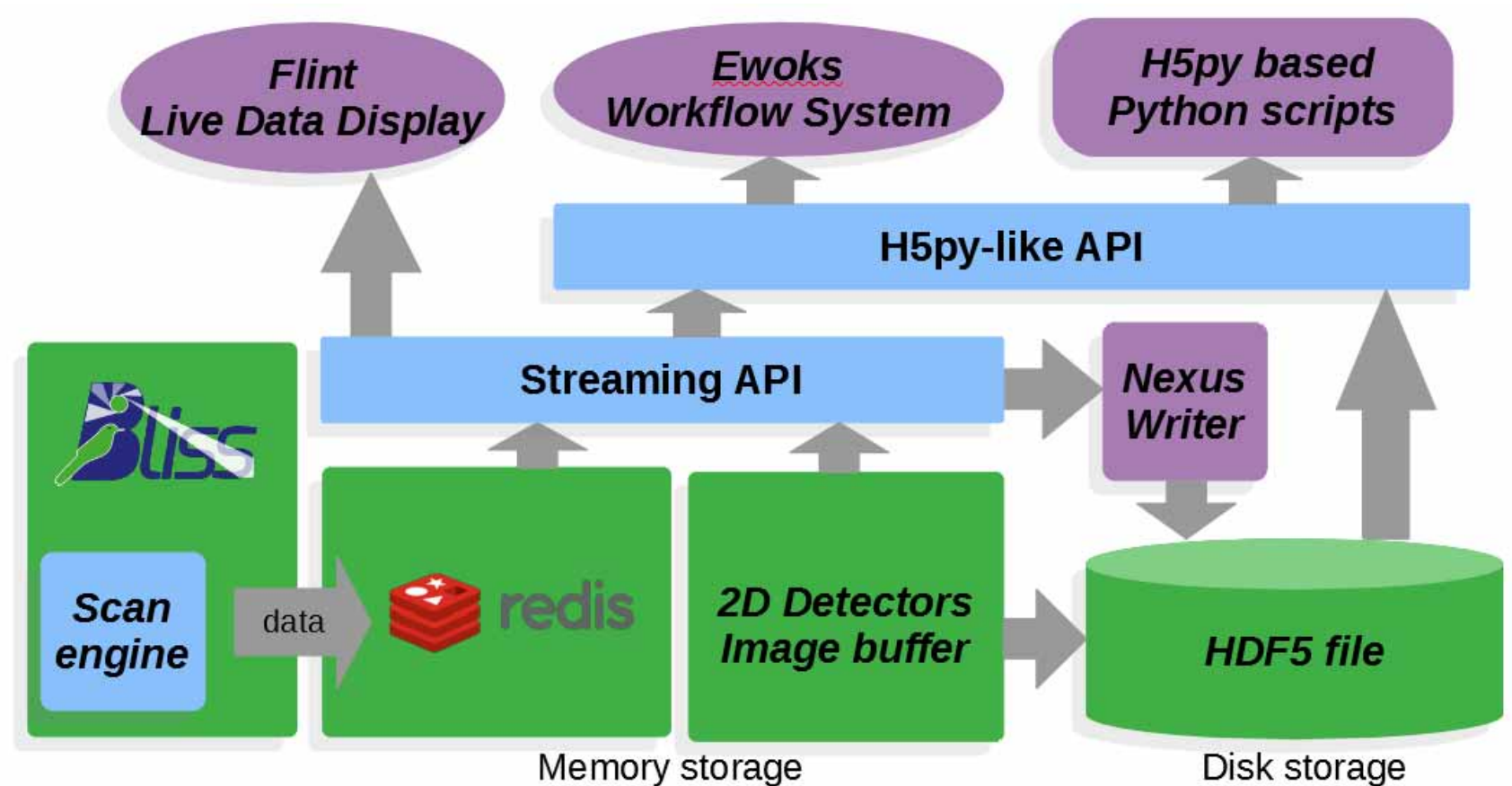
- **A generic scan engine** for step and continuous scans
The use of trajectories and HKL space is possible with all scans
- **Decoupling of data acquisition** from data saving and analysis
All data buffered in memory. Allows higher acquisition speed without blocking
- **Coherent HDF5 storage** of all acquired data at high speed and for large data volumes
All data of a proposal, its samples and the produced datasets is saved as a coherent HDF5 data tree
- **Live data display** of all acquired data
Immediate visibility of acquisition results for the user
- **Easy configuration** of hardware and experimental environment
Switch between predefined acquisitions set-ups on the fly
- **PyTango** to interface any device from the Tango world

BLISS is running in daily operation on 35 beamlines today!



TUSDSC01 BLISS: ESRF All-In-One, Python-based Experiment Control System

Data API for transparent on- and offline data access



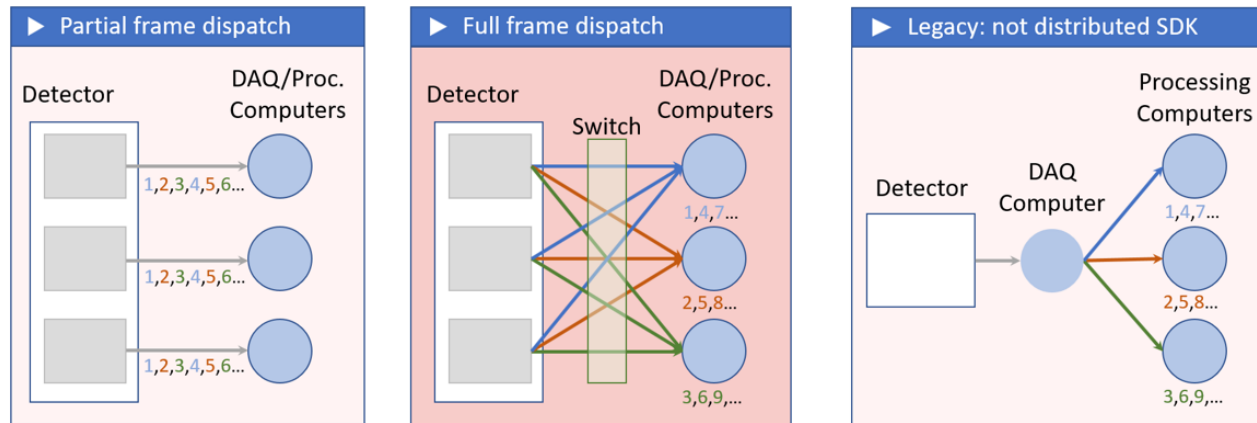
Distributed Acquisition for High Performance 2D Detectors

Multiple distributed receivers

Scalability for increasing data flows

Low latency image processing (CPU or GPU) on the data acquisition computers

- Online data reduction for large data volumes
- Closed loop applications with fast feedback to the experiment



Several topologies to distribute acquired images for processing

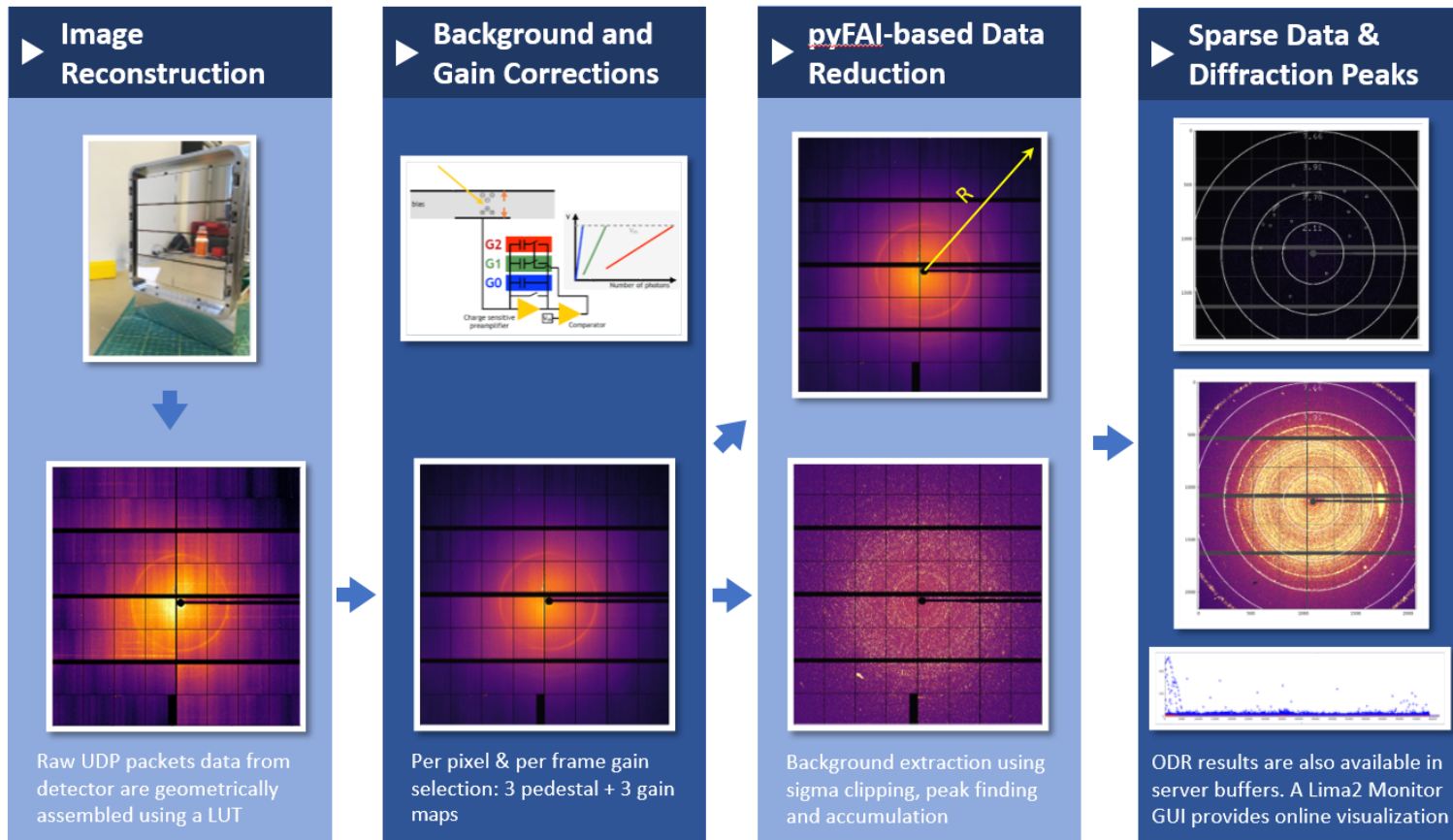


THMBCMO31 LIMA2: Towards a Distributed Acquisition and Processing Framework for High Performance 2D Detectors

Data Reduction Example

PSI Jungfrau 4M detector acquiring at 1kHz

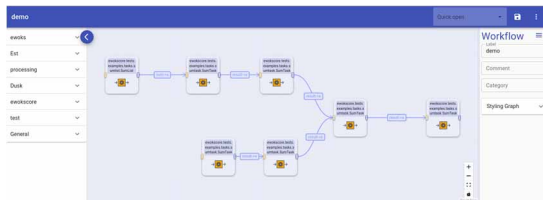
8GB/s of raw data reduced to 400 MB/s of sparse data



Ongoing processing pipeline optimization from 500hz to 1KHz

Workflow System for Online Data Analysis and Reduction

- **Graphical chaining** of predefined processing tasks by the user
- **Web GUI** to build workflows



- Specific **workflow tasks** for every scientific domain
- Can run **fully automated** or manually
- Processing by **CPU or GPU**, locally or batch cluster
- Results can be **stored or fed back** to the acquisition system

ESRF Workflow System (Ewoks)

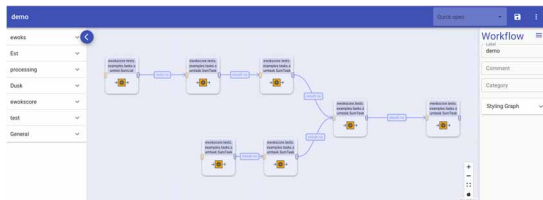
Beamlines using Ewoks

25 beamlines use Ewoks to process their data!
Discover 399 workflow tasks below or use the search on the left.

Tomography BM05, BM18, ID11, ID16B, ID17, ID19 30 tasks	SAXS/WAXS BM02, ID09, ID11, ID31 18 tasks	Spectroscopy BM23, ID24 15 tasks
Fluorescence ID16A, ID16B, ID21 11 tasks	Dark-field Microscopy ID06, ID11 16 tasks	Imaging ID16b, ID21 4 tasks
MX Beamline Automation ID23-1, ID23-2, ID30A-1, ID30A-3, ID30B 292 tasks	BioSAXS BM29 <i>Under construction</i>	Special Diffraction ID11, ID22 5 tasks
Special Spectroscopy ID26 <i>Under construction</i>	Data Access 0 tasks	Demo 8 tasks
Development BM16, ID10 <i>Under construction</i>		

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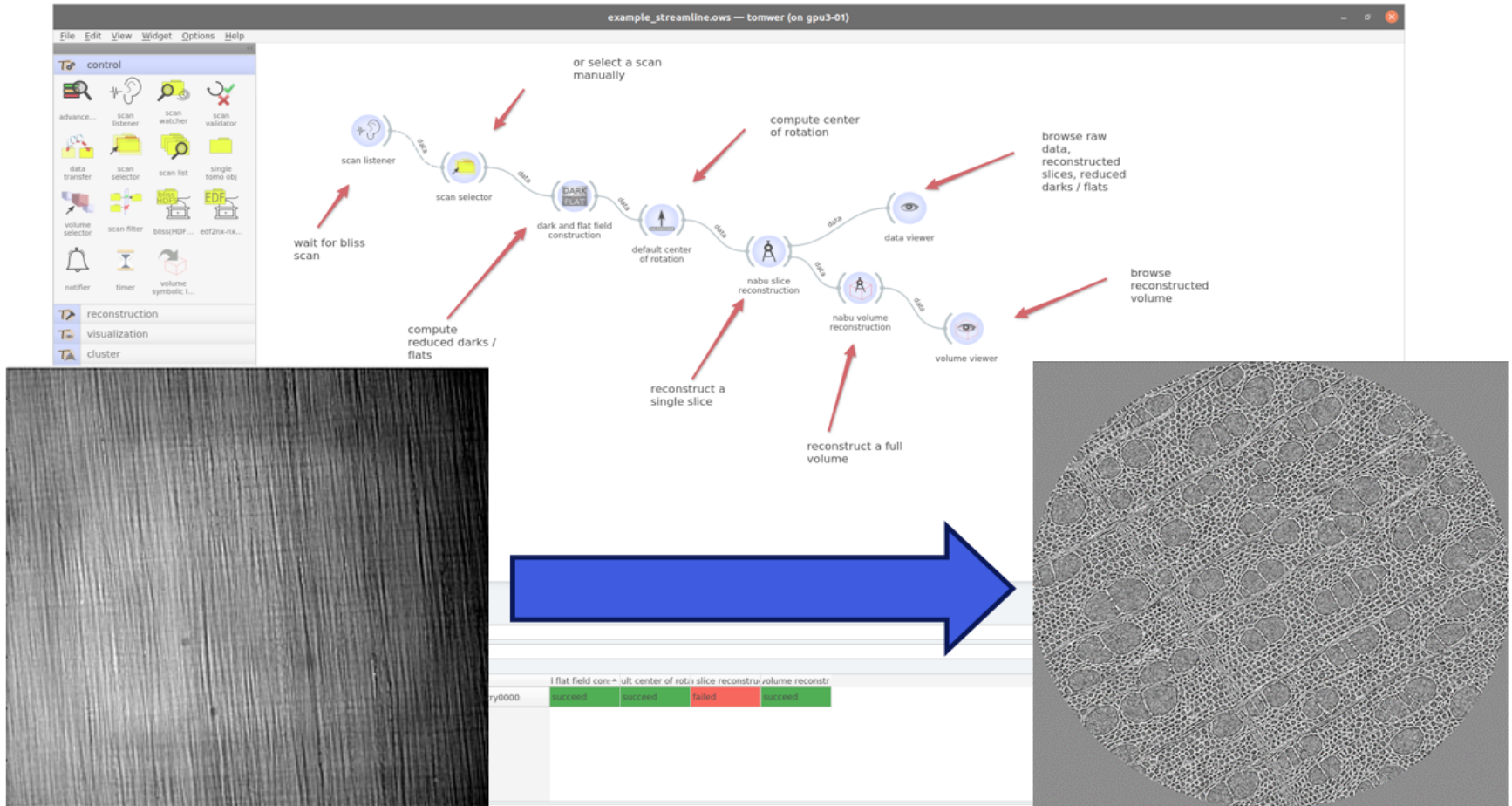
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EWOKS is running in daily operation on 25 beamlines today!

Tomography reconstruction (ID19, BM05, BM18, ID11, ID16B)

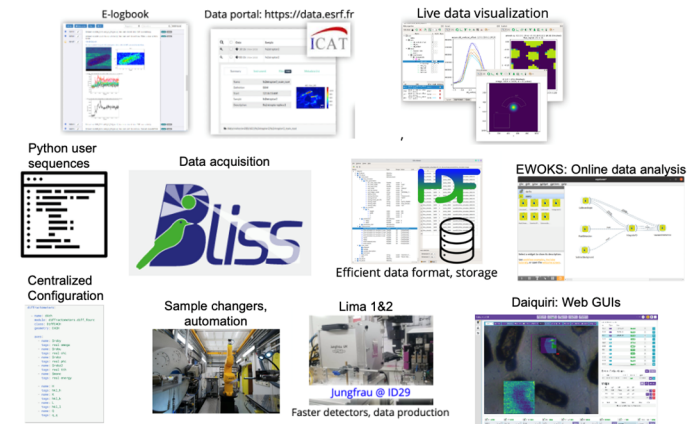


Inputs: BLISS scan data (darks, flats, projections + metadata)

Outputs: reconstructed volumes

BLISS and LIMA2

- Ready to push-up the data acquisition frequency
- Easy integration of user software
- High flexibility to prepare complex experiments
- Online data visualization
- Low latency image processing



Data management

- HDF5 saving structure, following the ESRF data policy, for all experiments
- Transparent online and offline data access for data analysis

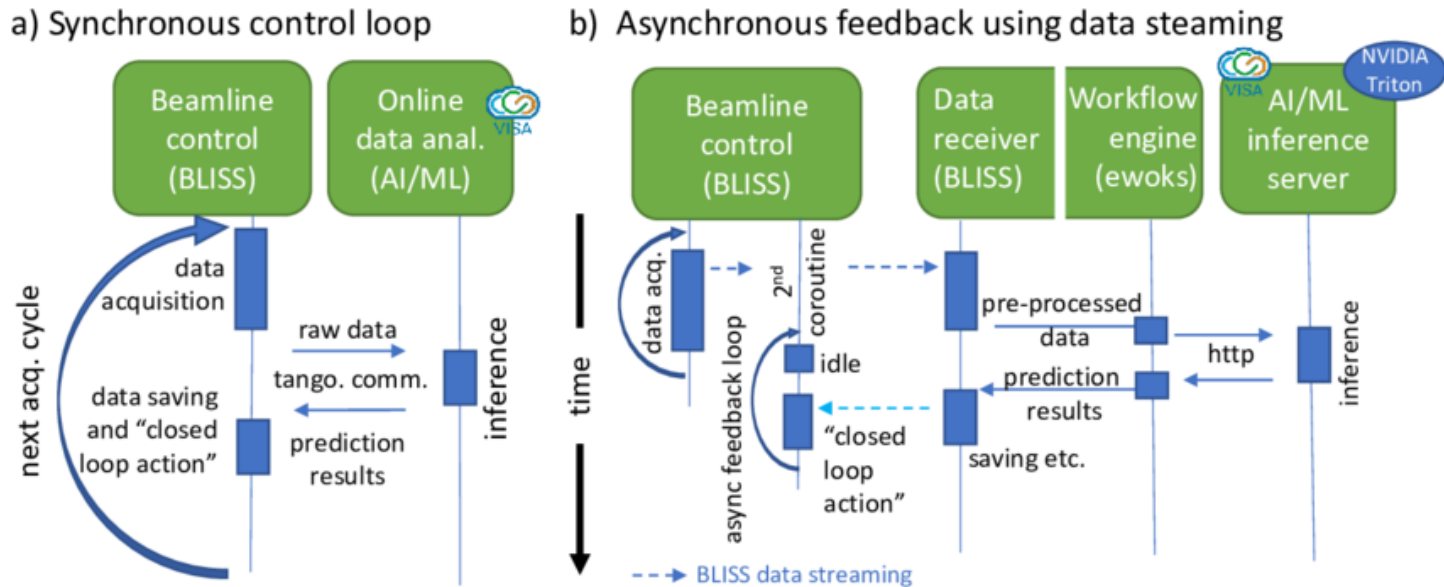
EWOKS

- Workflow definitions for different science domains
- Easy automation of data reduction and online processing
- Result feedback to the running acquisition

THE PROOF IS IN THE PUDDING

With BLISS, LIMA2, EWOKS and Tango the door is wide open for complex experiments

Example on ID10: Using AI/ML to close the loop with the running experiment




L.Pithan - Closing the loop: Autonomous experiments enabled by machine-learning-based online data analysis in synchrotron beamline environments



Acknowledgements to

- The members of the software group for the development of all the different software tools
- Our colleagues from the Technical Infrastructure Division for their work on the network and data storage infrastructure
- All the beamline scientists for their feedback, patience and bug reports since the EBS start-up

 **Bliss demo session:** https://bliss.gitlab-pages.esrf.fr/bliss/master/bliss_demo.html